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using LANL's D-Wave 2X

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Simulations of non-local spin interaction in atomic magnetometers using LANL's D-Wave 2X

Igor Savukov and Alexander Malyzhenkov

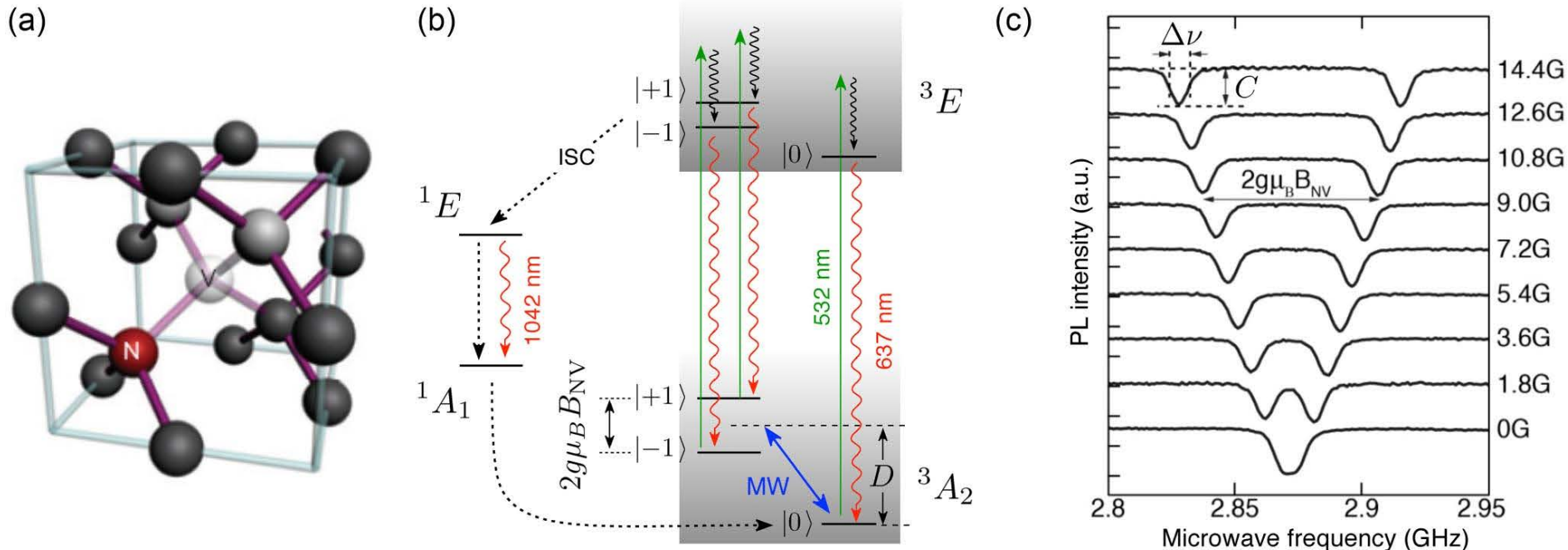
4/27/2017

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Nitrogen-vacancy (NV) defect in diamond

$$H = \hbar D S_z^2 + \hbar E (S_x^2 - S_y^2) + g \mu_B \mathbf{B} \mathbf{S} + H_d$$



[1] Rep. Prog. Phys. **77** (2014) 056503 (26pp)

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Simplifications of the Hamiltonian

$D \sim 2.87 \text{ GHz}$ or 100 mT

$E \sim 100 \text{ kHz}$ and can be neglected

$H_d \sim 100 \text{ mT}$ for 1 nm , or 0.1 mT for 10 nm .

$\hbar D S_z^2$ is not sensitive to the direction and does not play any role in our analysis when we consider only z component; however, forces the spin to be parallel to z .

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Ensemble of NV defects:

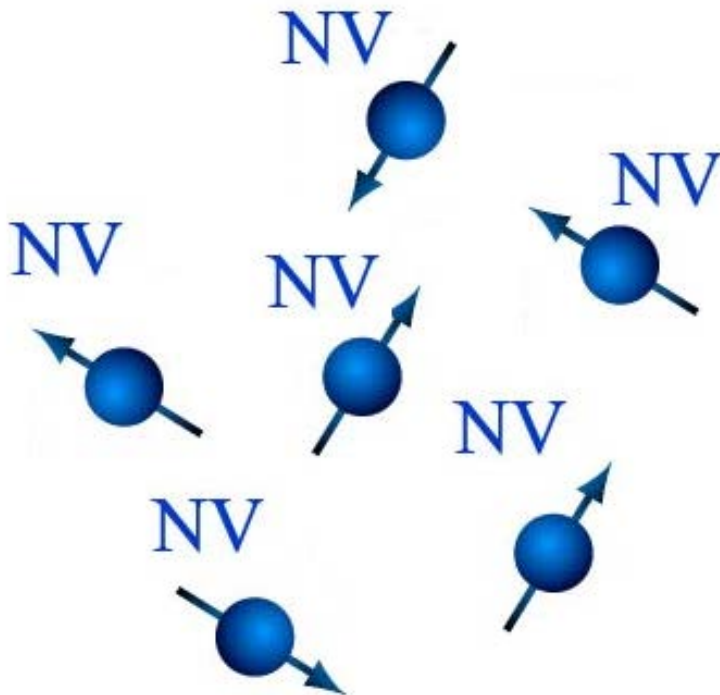
Signal to noise ratio for independent NV-centers:

$$SNR \sim \frac{1}{\sqrt{N}}$$

But dipole interaction between different NV-centers will also impact sensitivity and orientation of spins

$$H_i = - \sum \mathbf{m}_{NV_i} \mathbf{B}_{NV_j}$$

$$\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A} = \frac{\mu_0}{4\pi} \left(\frac{3\mathbf{r}(\mathbf{m} \cdot \mathbf{r})}{r^5} - \frac{\mathbf{m}}{r^3} \right)$$



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Ising part of the Hamiltonian

Spin-spin interaction with random positioning is extremely hard problem for classical computer, but it seems to be an ideal fit for Ising Quantum Computer such as D-Wave

Approximation: spin and magnetic field only along/opposite with z-axis; however, it can be justified for stationary states

$$H = \sum_i k_1 s_i B(r_i) + \sum_i \sum_{j < i} 2k_2 s_i s_j / r_{ij}^3 (1 - \frac{3z_{ij}^2}{r_{ij}^2})$$

$$r_{ij} = \sqrt{(i_x - j_x)^2 + (i_y - j_y)^2 + (i_z - j_z)^2}; z_{ij} = (i_z - j_z)$$

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Ground and excited states

To understand the dynamics of NV-diamond spins, the ground state is not sufficient and excited states also need to be found.

D-Wave finds automatically the ground state or low-excited states when the temperature is finite and the thermal energy is comparable to the splitting.

A more reliable method to find excited states is to introduce penalty energy for a state of being non-orthogonal to the ground state

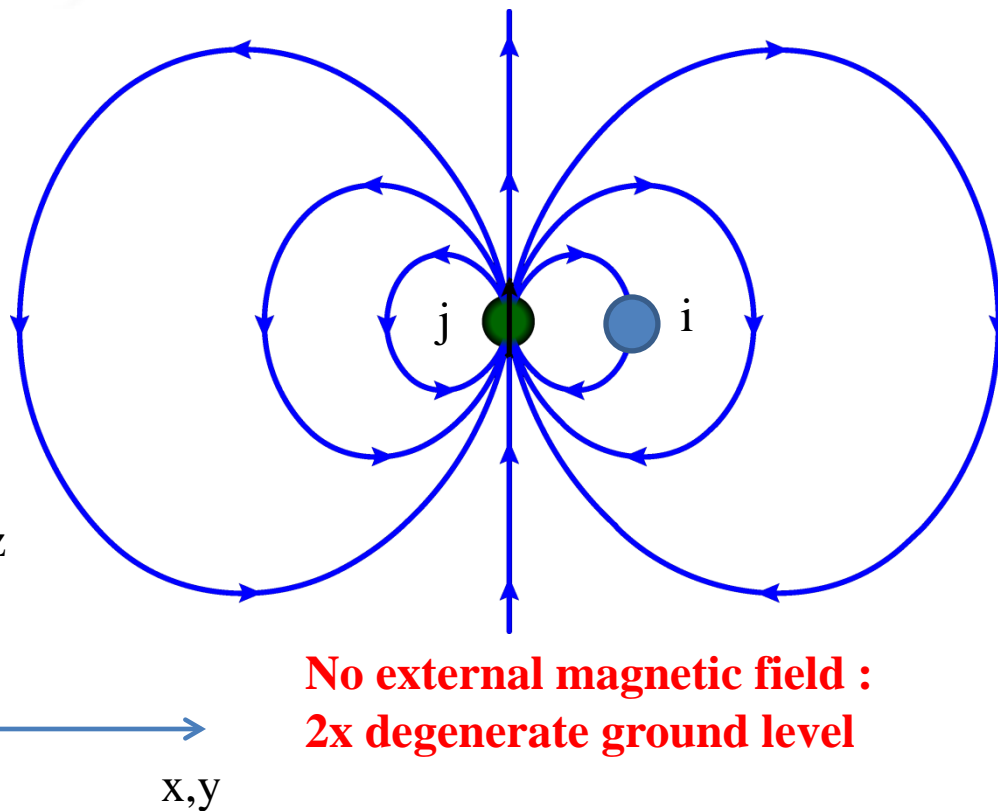
$$H = k_3 \sum_i s_i^{gr} s_i, k_3 > 0$$

This term can be combined with the Zeeman single-sum term and the new “ground” state, orthogonal to the real one is found by D-Wave. This process can be continued by adding the term enforcing orthogonality with the first excited states, and so on.

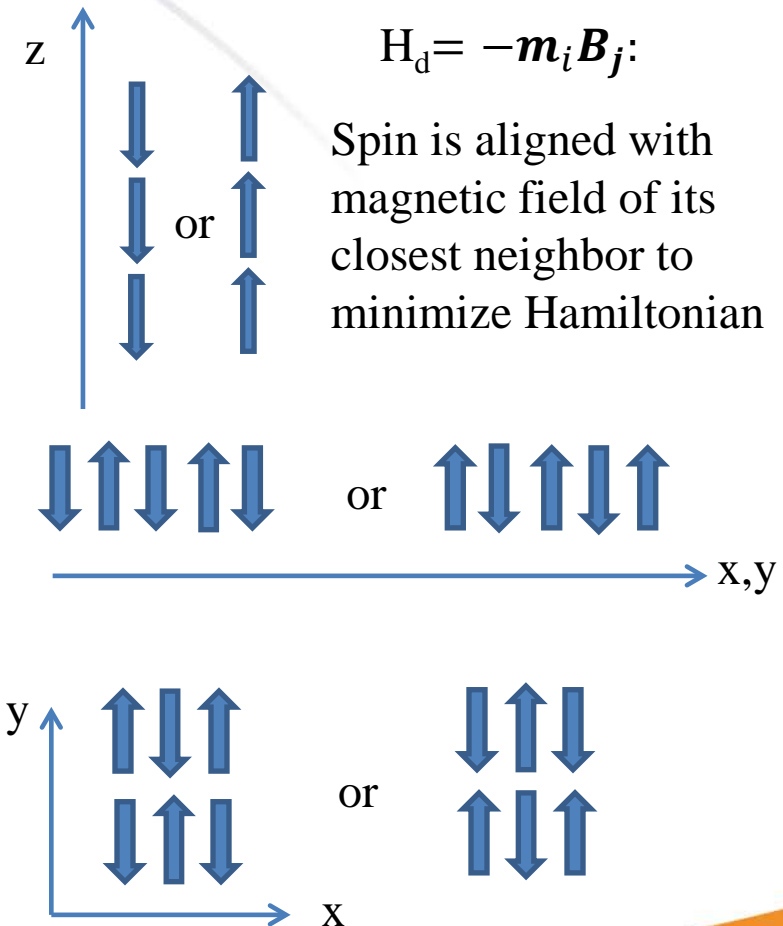
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Dipole field map to predict solutions

We can predict solutions in some trivial spin configurations



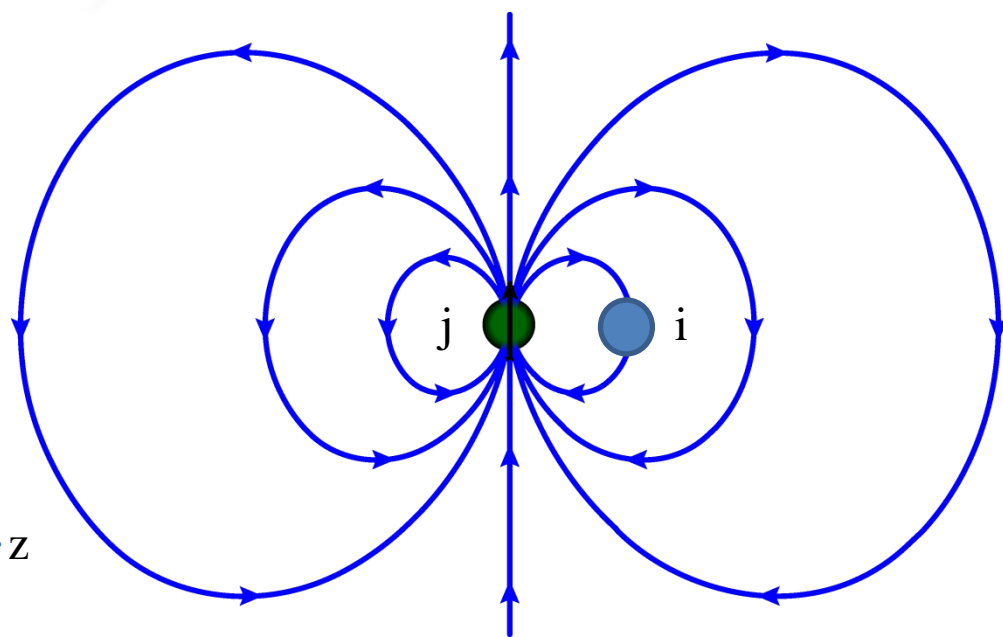
**No external magnetic field :
2x degenerate ground level**



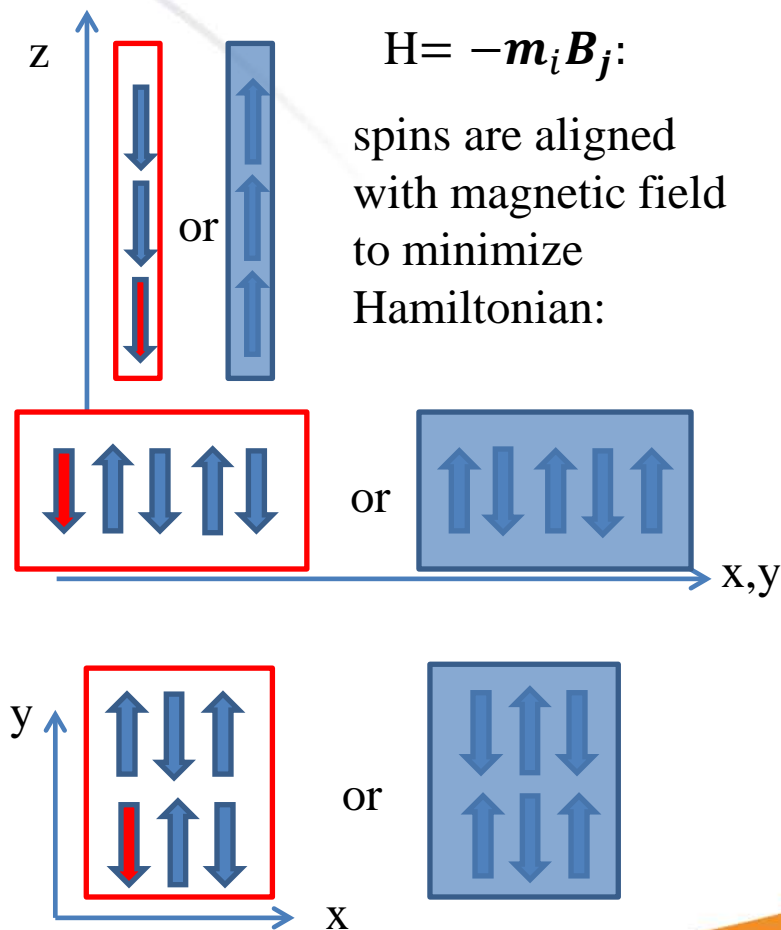
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Dipole field map to predict solutions

We can predict solutions in some trivial spin configurations



First spin is fixed down by strong magnetic field: selecting one solution



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Is **D-Wave 2X** capable to find energy levels (*at least ground state*) of many (*how many?*) NV-diamond spins system in our approximation?

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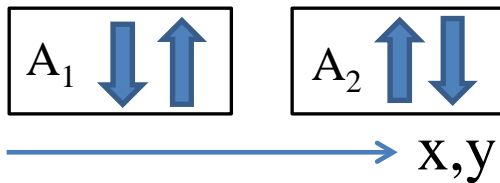
Problems we found

1. **D-Wave 2X bias:** spin up and spin down are not the same
2. **Embedding:**
 - a) increasing the number of spins in the system requires a lot of couplings, which squeezes the dynamic range
 - b) only 45 spins connected to each other are possible to simulate on **D-Wave 2X** unless we “cheat” and cut long distance interaction

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2-spin system (x/y-line): no embedding needed

*Expectations:
50% and 50%*



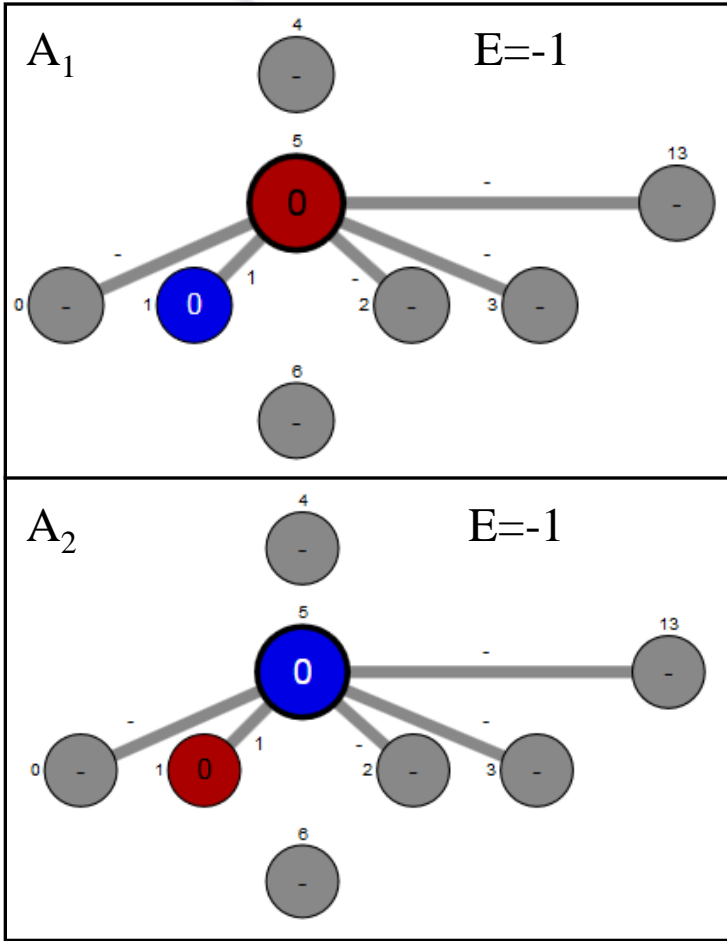
Samples=1000

Run	1	2	3	4	5	Total
A_1	565	570	474	612	440	2661
A_2	435	430	526	388	560	2339

Classical computer states to compute E and sort*: $n=2^2=4$

**Quick sort:*
 $D_{min}=n \log(n)$
 $D_{max}=n^2$

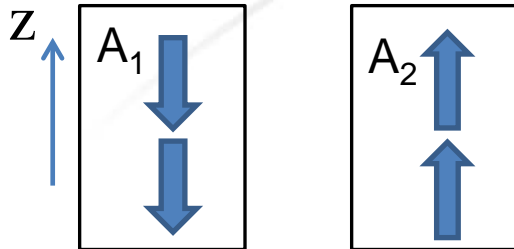
D-Wave solutions:



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2-spin system (z-line): no embedding needed

*Expectations:
50% and 50%*



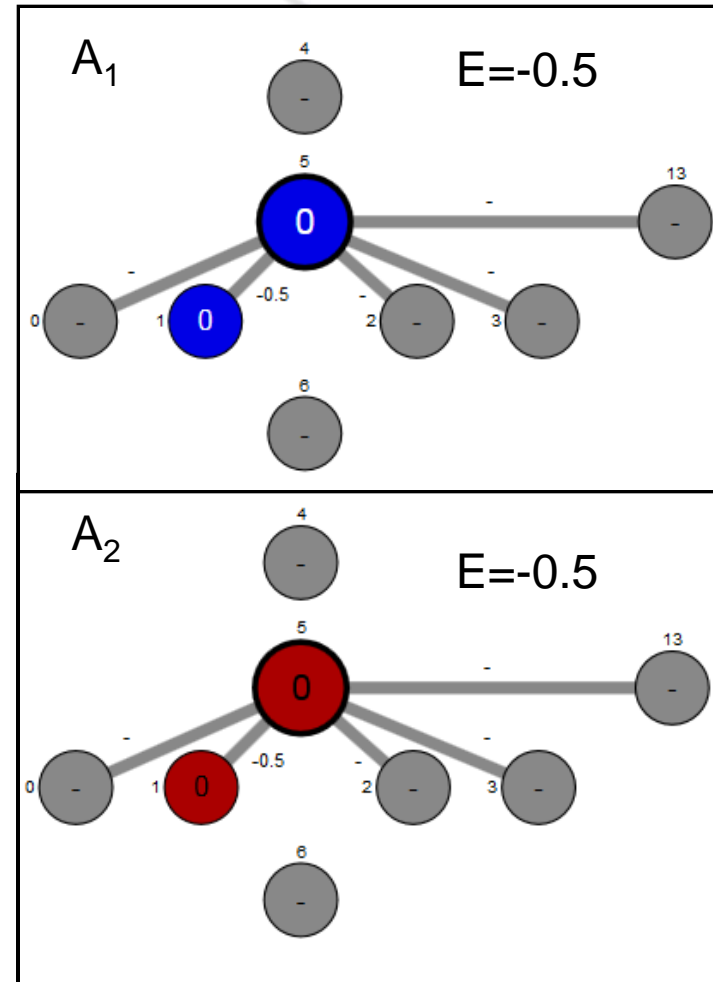
Samples=1000;

Bias?



Run	1	2	3	4	5	Total
A_1	714	626	683	755	658	3436
A_2	286	374	317	245	342	1564

D-Wave solutions:

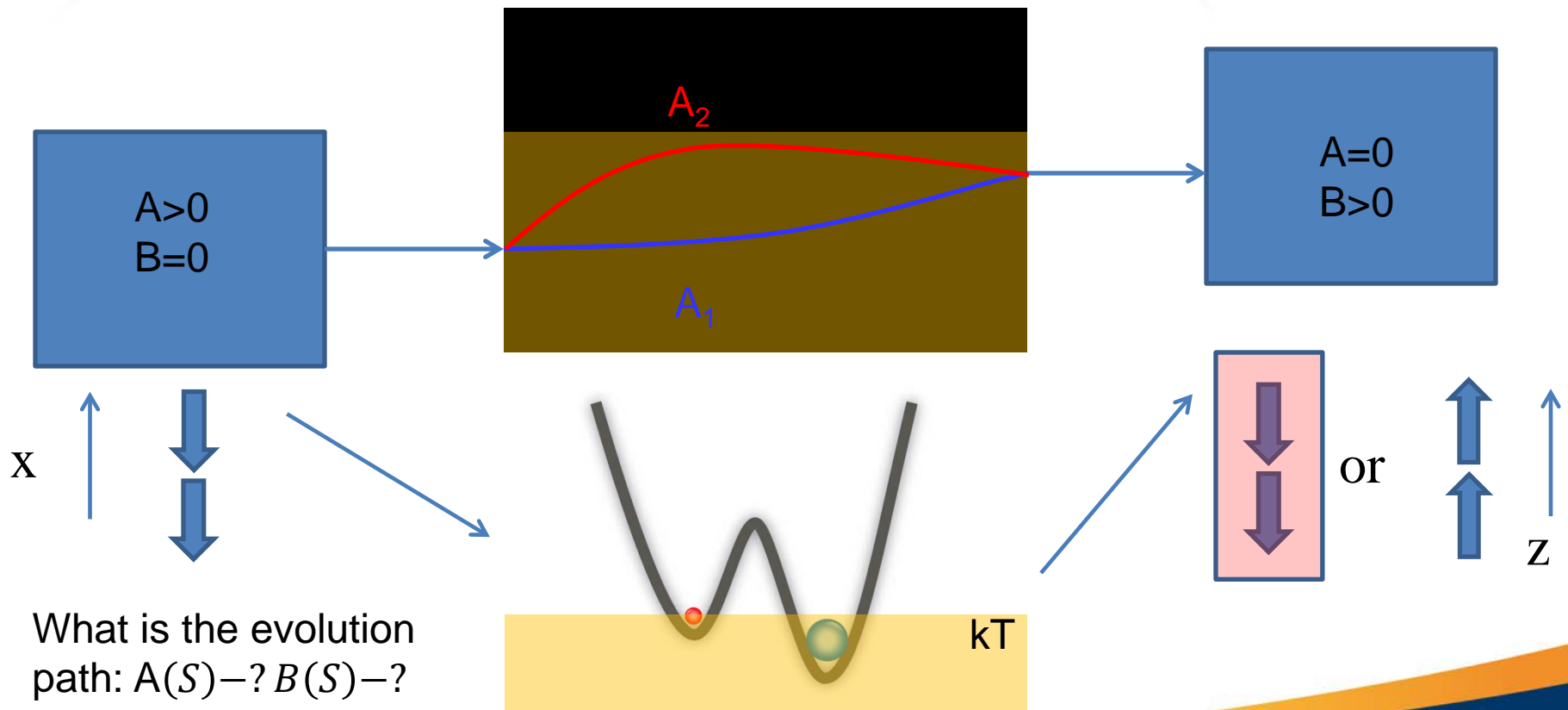


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Bias: adiabatic DWAVE evolution

$$E_{ising}(s) = \frac{A(s)}{2} \left(\sum_i \sigma_x^{(i)} \right) + \frac{B(s)}{2} \left(\sum_i h_i \sigma_z^{(i)} + \sum_{i>j} J_{i,j} \sigma_z^{(i)} \sigma_z^{(j)} \right)$$

Bias dependence from temperature (annealing time) will be an interesting problem to study

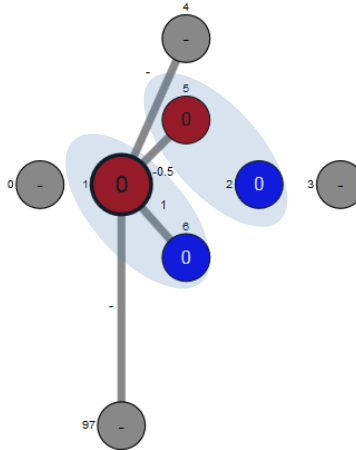


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How to get right solutions with biased D-Wave

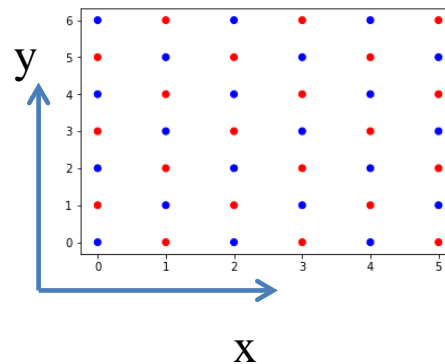
1. Spin anti-cloning

*Problem: squeezing dynamic range **



Anti-cloning based embedding would be ideal for systems which need embedding anyway
**dynamic range would be the same as in regular embedding*

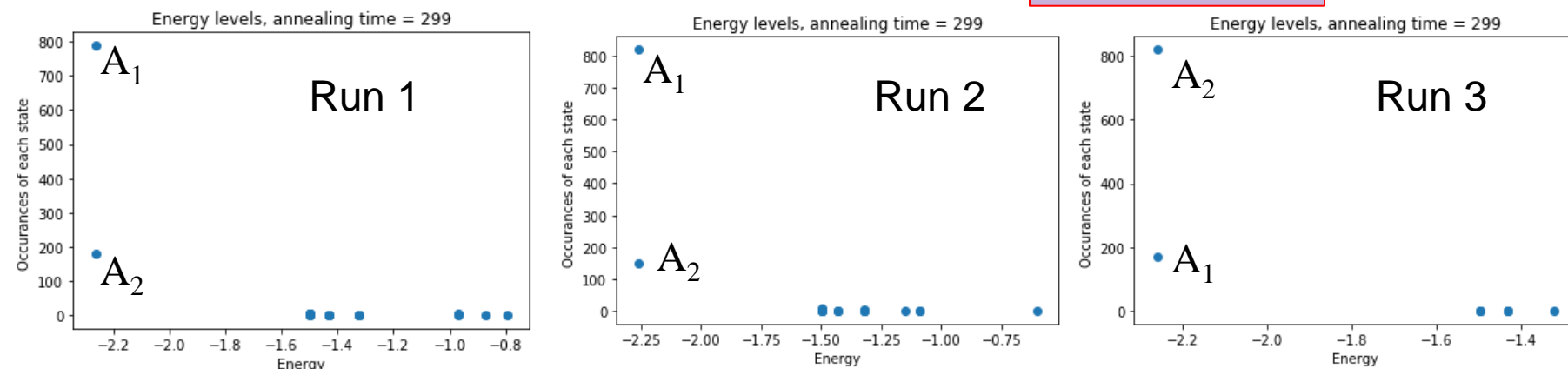
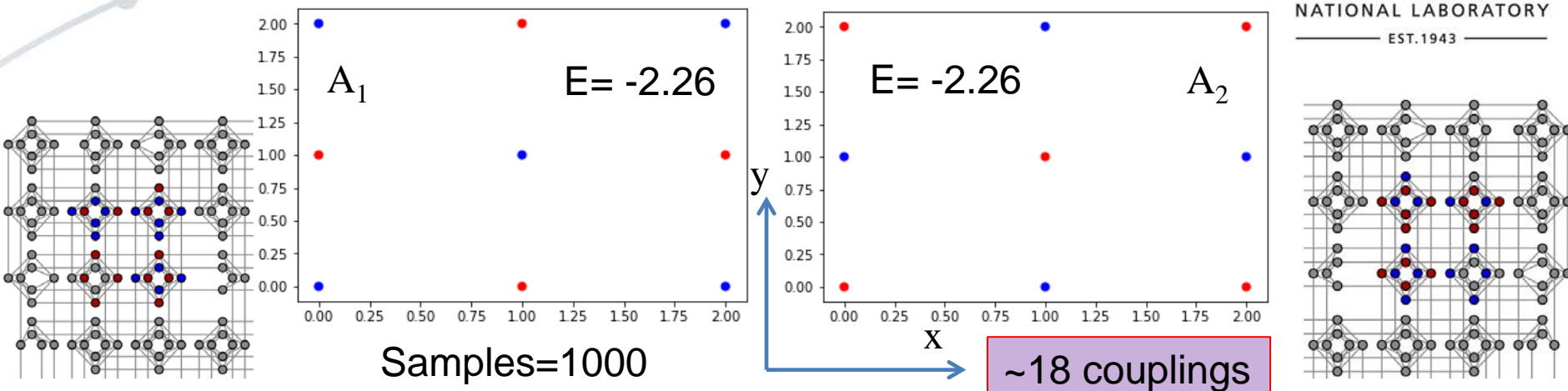
2. Choosing symmetrical relatively to spin direction systems to study



For such symmetrical systems all embedding chains should be ideally of the same length

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2D spin system: $9=3*3$ spins

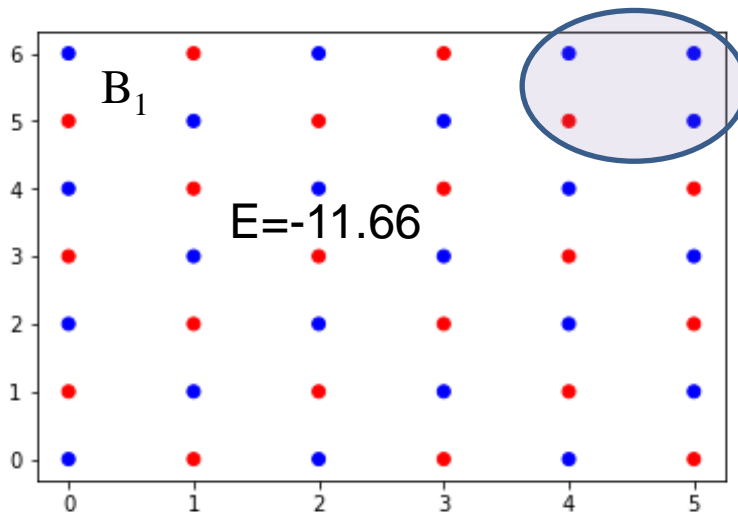
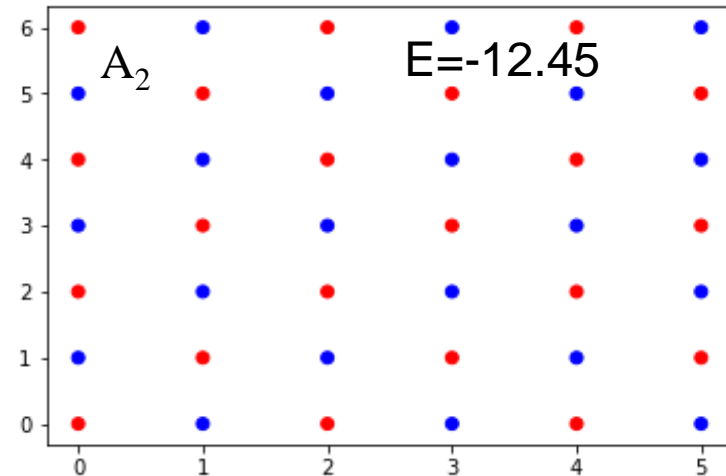
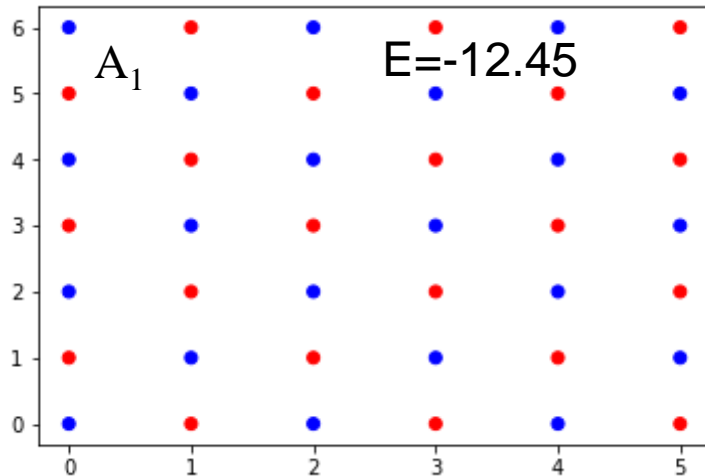


Classical computer
states to compute E
and sort*: $n=2^9=512$

*Quick sort:
 $D_{min}=n \log(n)$
 $D_{max}=n^2$

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2D spin system: $42=6*7$ spins



Spin flip

~800 couplings

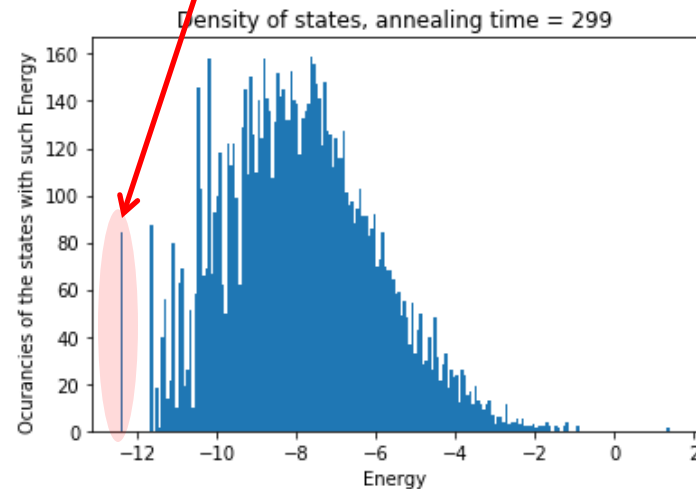
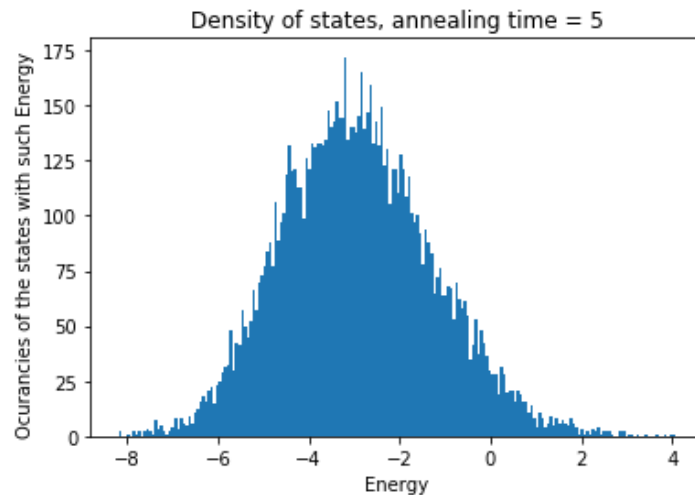
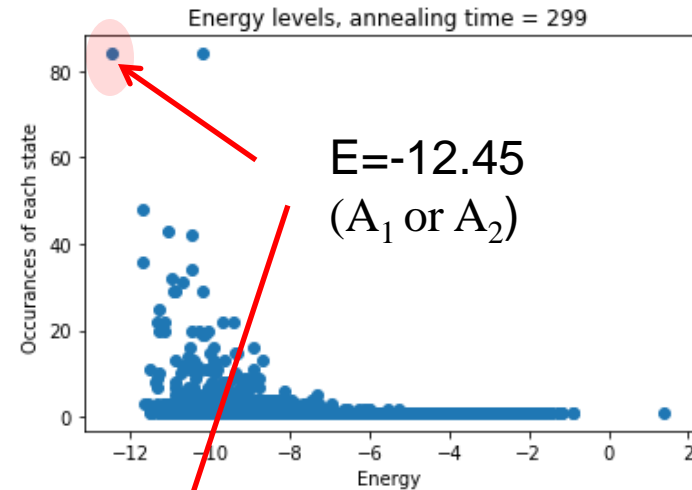
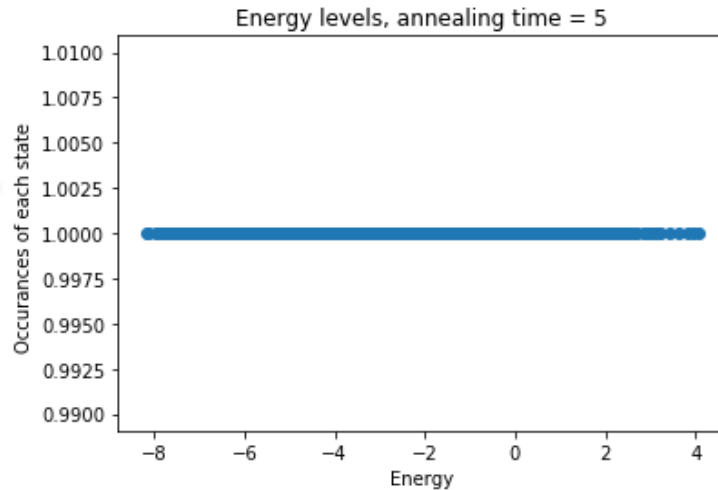
Classical computer
states to compute E and
sort*: $n=2^{42} \sim 4*10^{12}$

*Quick sort:
 $D_{min}=n \log(n)$
 $D_{max}=n^2$

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Annealing time dependence

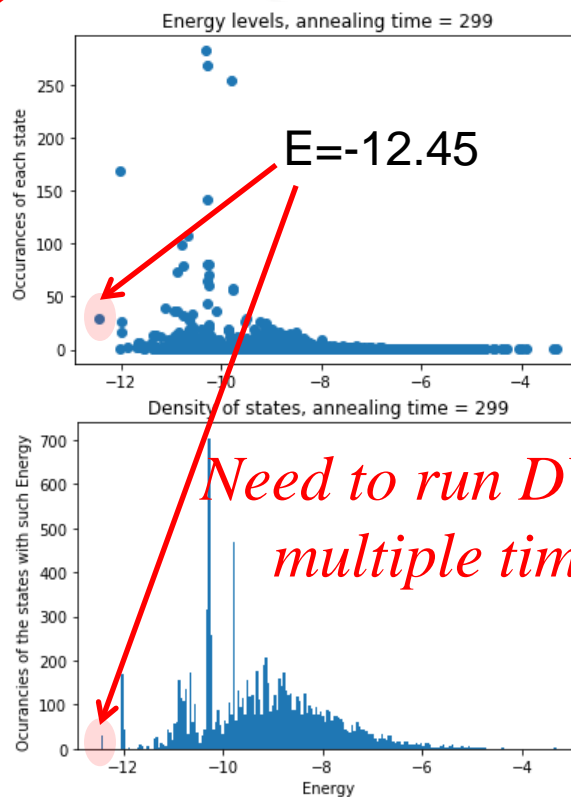
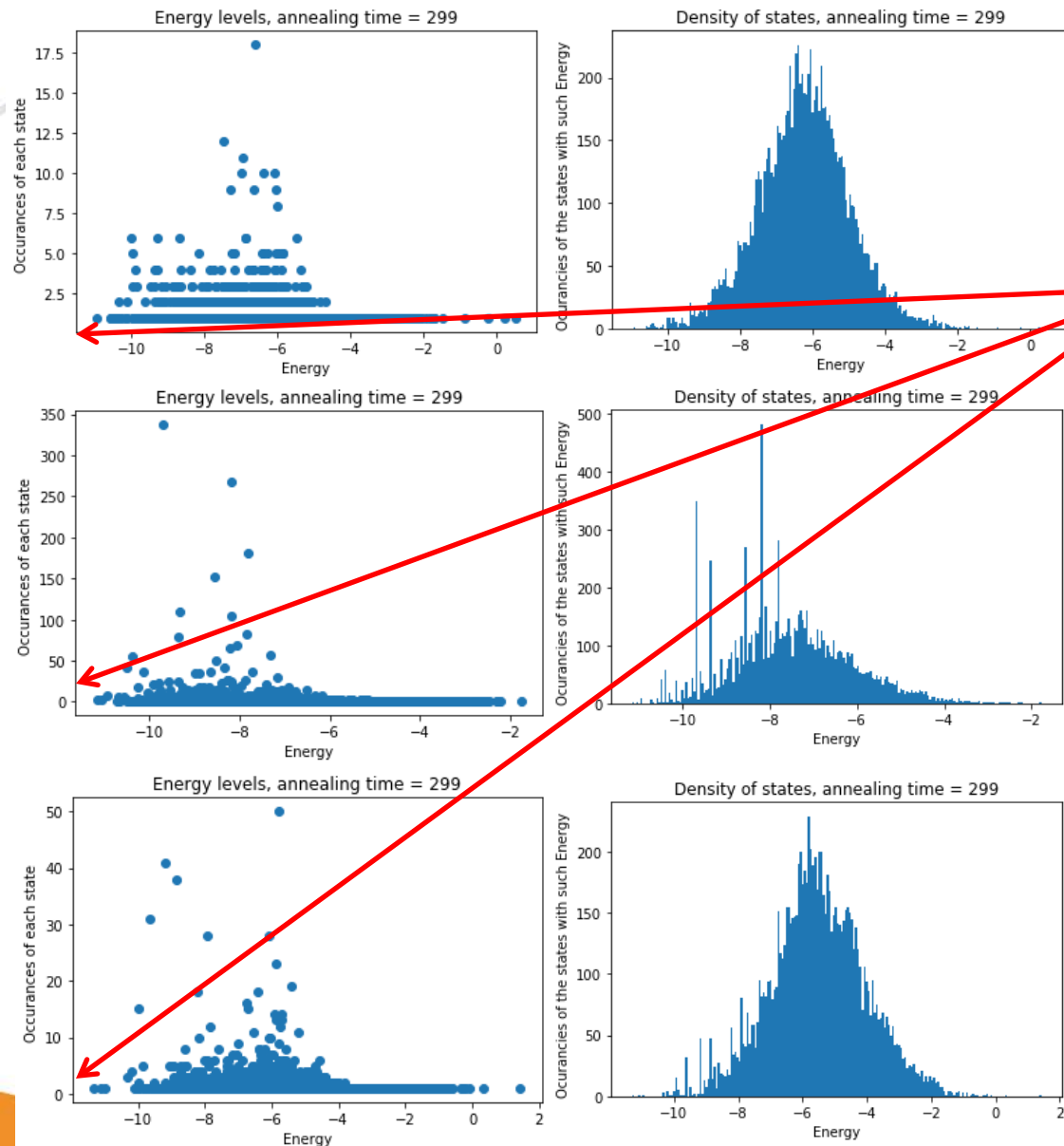
42 spins, samples=10000



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Same parameters – different results

Missing ground level
solution 3 times from 4

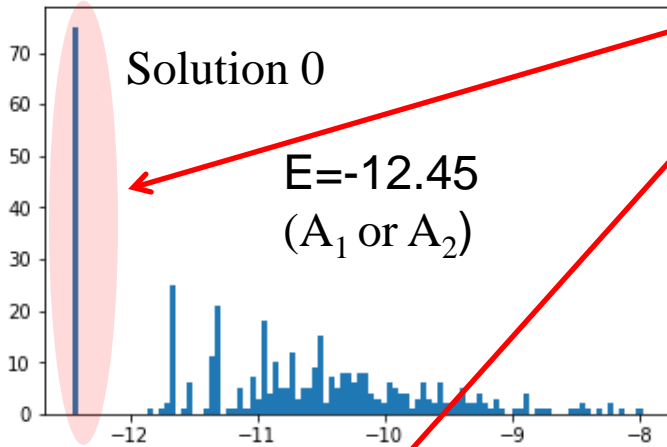


Annealing time dependence: multiple runs

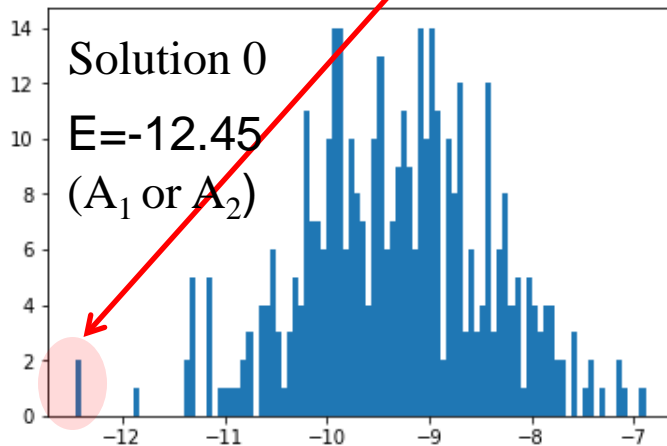
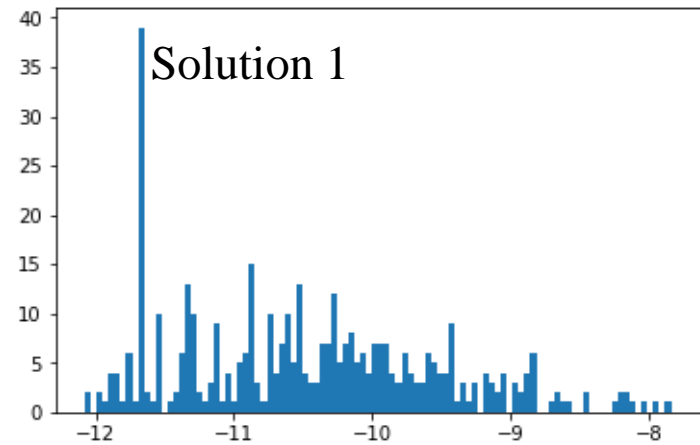
Only analyzing two first (lowest energy) levels from DWAVE each run:

[runs=400, samples=10000]

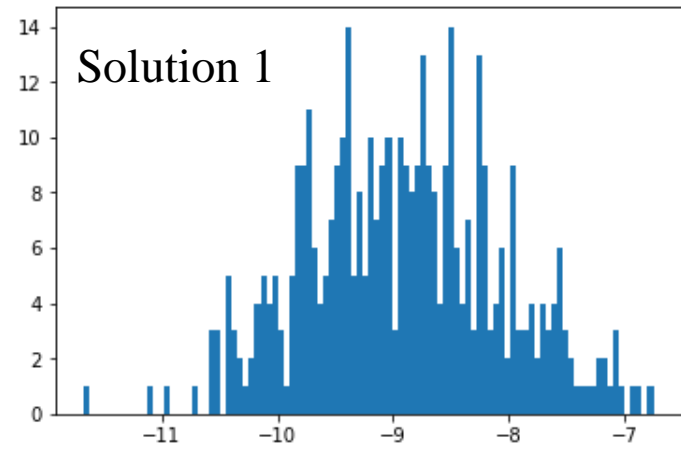
Solution 0 and 1 should have the same energy ~ -12.45 , but we find only "0" in ground state



**Annealing
time = 299**



**Annealing
time = 5**



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